```
chain nodes :
   18 21
ring nodes :
   1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
   2-18 5-8 7-14 11-21
ring bonds :
   1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16
   16-17
exact/norm bonds :
   1-2 1-6 2-3 2-18 3-4 4-5 5-6 7-8 7-11 7-14 8-9 9-10 10-11
exact bonds :
   5-8 11-21
normalized bonds :
   12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
   containing 1 : 7 : 12 :
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
   12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS
Generic attributes :
                            : Unsaturated
    Saturation
   Number of Carbon Atoms : less than 7
   Type of Ring System : Monocyclic
Element Count :
   Node 18: Limited
       C, C4-5
       N, N1-2
       0,00
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S,S0

Uploading C:\Program Files\Stnexp\Queries\10588876.str

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0,00 S,S0

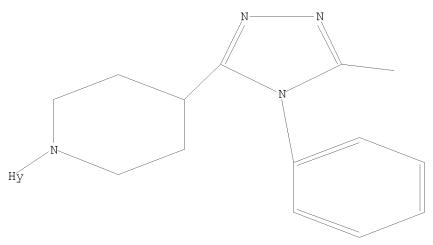
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chain nodes :
18 21
ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
          7-14 11-21
2-18 5-8
ring bonds :
1-2^{-1} 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 \quad 1-6 \quad 2-3 \quad 2-18 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 7-14 \quad 8-9 \quad 9-10 \quad 10-11
exact bonds :
5-8 11-21
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1:7:12:
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS
Generic attributes :
18:
                        : Unsaturated
Saturation
Number of Carbon Atoms : less than 7
Type of Ring System
                       : Monocyclic
Element Count :
Node 18: Limited
    C,C4-5
    N, N1-2
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L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 14:56:25 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 101 TO ITERATE

100.0% PROCESSED 101 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1418 TO 2622 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> => s 11 sss ful

FULL SEARCH INITIATED 14:56:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1737 TO ITERATE

100.0% PROCESSED 1737 ITERATIONS 21 ANSWERS

SEARCH TIME: 00.00.01

L3 21 SEA SSS FUL L1

=> => s 13

L4 2 L3

 \Rightarrow d 14 1-2 bib, ab, hitstr

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ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
T.4
     2005:962050 CAPLUS
ΑN
DN
     143:266931
     Preparation of triazoles which inhibit vasopressin antagonistic activity
ΤI
ΙN
     Bryans, Justin Stephen; Johnson, Patrick Stephen; Ryckmans, Thomas;
     Stobie, Alan
PA
     Pfizer Limited, UK; Pfizer Inc.
     PCT Int. Appl., 55 pp.
SO
     CODEN: PIXXD2
                                                  Applicant's
DT
     Patent
     English
LA
FAN.CNT 1
                         KIND DATE
     PATENT NO.
                                          APPLICATION NO.
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     WO 2005079808
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              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
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                                  20061106
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     US 2007203132
                          A1 20070830
                                                                        20070129
PRAI GB 2004-1384
                          Α
                                20040122
     US 2004-549407P
                          Р
                                20040301
     WO 2005-IB79
                          W
                                20050111
     WO 2005-IB9
                           W
                                  20050111
OS
     MARPAT 143:266931
AB
     The title compds. I [Het = 2-pyridinyl or 2-pyrimidinyl; R1 = H, alkyl or
     a nitrogen-containing heterocyclic ring having 5-6 ring atoms; R2 = H, benzyl
     or alkyl; and R3 = H, Me, OMe or Cl], useful for treating anxiety,
     cardiovascular disease (including angina, atherosclerosis, hypertension,
     heart failure, edema, hypernatremia), dysmenorrhea (primary and
     secondary), endometriosis, emesis (including motion sickness),
     intrauterine growth retardation, inflammation (including rheumatoid
     arthritis), mittelsmerchz, preclampsia, premature ejaculation, premature
     (preterm) labor and Raynaud's disease, were prepared Thus, heating
     2-[4-(5-methyl-[1,3,4]oxadiazol-2-yl)piperidin-1-yl]pyrimidine (preparation
     given) with 2-ethylphenylamine in the presence of MgC12 in a sealed vessel
     at 150\,^{\circ}\text{C} for 18 h afforded I [Het = 2-pyrimidinyl; R1 = H; R2 = Et; R3 = H]. All the exemplified compds. I showed a Ki of less than 400 nM
     when tested in screen 1.0 (V1A filter binding assay).
     863780-52-3P 863780-53-4P 863780-54-5P
     863780-55-6P 863780-56-7P 863780-57-8P
     863780-58-9P 863780-59-0P 863780-60-3P
     863780-61-4P 863780-62-5P 863780-63-6P
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863780-64-7P 863780-65-8P 863780-66-9P 863780-68-1P 863780-69-2P 863780-71-6P

863780-72-7P 863780-73-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of triazoles which inhibit vasopressin antagonistic activity)

RN 863780-52-3 CAPLUS

CN Pyrimidine, 2-[4-[4-(2-ethylphenyl)-5-methyl-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-53-4 CAPLUS

CN Pyrimidine, 2-[4-[5-methyl-4-(2-propylphenyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-54-5 CAPLUS

CN Pyrimidine, 2-[4-[5-methyl-4-[2-(1-methylethyl)phenyl]-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-55-6 CAPLUS

CN Morpholine, 4-[[4-phenyl-5-[1-(2-pyrimidinyl)-4-piperidinyl]-4H-1,2,4-triazol-3-yl]methyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \\ & & \\ N & \\ \end{array}$$

RN 863780-56-7 CAPLUS

CN Pyrimidine, 2-[4-(5-butyl-4-phenyl-4H-1,2,4-triazol-3-yl)-1-piperidinyl]- (CA INDEX NAME)

RN 863780-57-8 CAPLUS

CN Pyrimidine, 2-[4-[4-phenyl-5-(1-piperidinylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-58-9 CAPLUS

CN Pyrimidine, 2-[4-(5-methyl-4-phenyl-4H-1,2,4-triazol-3-yl)-1-piperidinyl]- (CA INDEX NAME)

RN 863780-59-0 CAPLUS

CN Pyridine, 2-[4-[4-(4-methoxy-2-methylphenyl)-5-methyl-4H-1,2,4-triazol-3-

yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-60-3 CAPLUS

CN Pyridine, 2-[4-[4-(4-chloro-2-methylphenyl)-5-methyl-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-61-4 CAPLUS

CN Pyridine, 2-[4-[5-methyl-4-(2-methylphenyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-62-5 CAPLUS

CN Pyridine, 2-[4-[4-(4-chlorophenyl)-5-methyl-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-63-6 CAPLUS

CN Pyridine, 2-[4-[4-(4-methoxyphenyl)-5-(2H-1,2,3-triazol-2-ylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-64-7 CAPLUS

CN Pyridine, 2-[4-[4-(4-methoxyphenyl)-5-methyl-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-65-8 CAPLUS

CN Pyridine, 2-[4-[4-(2-methylphenyl)-5-(2H-1,2,3-triazol-2-ylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ N & \\$$

RN 863780-66-9 CAPLUS

CN Pyridine, 2-[4-[4-(4-chloro-2-methylphenyl)-5-(2H-1,2,3-triazol-2-ylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{Me} \\ \text{N} \\$$

RN 863780-68-1 CAPLUS

CN Pyridine, 2-[4-[4-phenyl-5-(2H-1,2,3-triazol-2-ylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & & & Ph \\ & & & \\ N & & N \\ \hline & N & & N \\ \hline & N & & N \\ \end{array}$$

RN 863780-69-2 CAPLUS

CN Pyridine, 2-[4-[4-(4-chlorophenyl)-5-(2H-1,2,3-triazol-2-ylmethyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

$$\begin{array}{c|c} C1 \\ \hline \\ N \\ \hline \\ N \\ \end{array}$$

RN 863780-71-6 CAPLUS

CN Pyridine, 2-[4-[5-methyl-4-(4-methylphenyl)-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-72-7 CAPLUS

CN Pyridine, 2-[4-[4-(2,4-dimethylphenyl)-5-methyl-4H-1,2,4-triazol-3-yl]-1-piperidinyl]- (CA INDEX NAME)

RN 863780-73-8 CAPLUS

CN Morpholine, 4-[[4-(4-chloro-2-methylphenyl)-5-[1-(2-pyridinyl)-4-piperidinyl]-4H-1,2,4-triazol-3-yl]methyl]- (CA INDEX NAME)

$$\begin{array}{c|c} C1 \\ \\ Me \\ \\ N \\ \\ N \\ \\ N \\ \\ N \\ \end{array}$$

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
T. 4
       2004:718543 CAPLUS
ΑN
      141:225517
DN
       Preparation of triazoles as vasopressin receptor V1a antagonists for
TI
       treating of dysmenorrhea
IN
       Bryans, Justin Stephen; Johnson, Patrick Stephen; Ryckmans, Thomas;
       Stobie, Alan
       Pfizer Limited, UK; Pfizer Inc.
PA
       PCT Int. Appl., 164 pp.
                                                                       common inventors
       CODEN: PIXXD2
DT
       Patent
LA
       English
FAN.CNT 2
                                 KIND
                                             DATE
                                                            APPLICATION NO.
       PATENT NO.
                                                                                               DATE
       WO 2004074291 A1 20040902 WO 2004-IB432
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       BR 2004007676 A 20060301 BR 2004-7676 20040209
      CN 1751047 A 20060322 CN 2004-80004708
JP 2006517921 T 20060803 JP 2006-500323
AT 349449 T 20070115 AT 2004-709303
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      AT 380048 T 20071215 AT 2004-743961
US 2005026810 A1 20050203 US 2004-895630
IN 2005DN03308 A 20070713 IN 2005-DN3308
MX 2005PA08923 A 20060309 MX 2005-PA8923
KR 750028 B1 20070816 KR 2005-715408
                                                                                               20040712
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      B1 20070816

NO 2005004053 A 20051031

US 2006194794 A1 20060831

JP 2007045838 A 20070222

GB 2003-3852 A 20030219

GB 2003-17227 A 20030723

US 2003-455455P P 20030318

US 2003-493823P P 20030808

JP 2006-500323 A3 20040209

WO 2004-IB432 W 20040205
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                                                            NO 2005-4053
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PRAI GB 2003-3852
                                         20030316
20030808
20040209
20040209
       US 2004-782285
                                   A3
                                         20040218
OS
      MARPAT 141:225517
      Title compds. I [wherein V = -(CH2)d(O)e-, -CO-, -CH(alkyl)-; W = O,
```

S(:0)a, NH and derivs.; X, Y = independently H, alkyl, halo, OH, CF3, OCF3, alkoxy, Z = -(CH2)f(O)g-, -CO-, -CH(alkyl)-; A = 4-7 membered (un)substituted saturated N-containing heterocycle; B = Ph, (un)substituted saturated

N-containing heterocycle; a = 0-2; e, g = 0-1; d, f = 1-2; and their pharmaceutically acceptable derivs.] were prepared as vasopressin receptor V1a antagonists for the treatment of dysmenorrhea. Thus, amination of chloride II (preparation given) with 2-aminomethyl-4-chlorophenylamine (preparation

given), cyclization of the aminooxadiazole, and reaction of amine with dimethylsulphamoyl chloride gave the triazole III. III displayed a $\rm Ki=0.24~nM$ in a V1a filter binding assay.

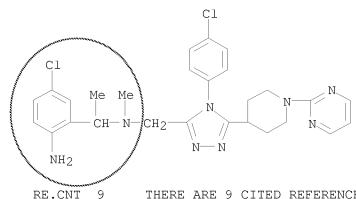
IT 748806-15-7P, [4-Chloro-2-[1-[[[4-(4-chlorophenyl)-5-[1-(pyrimidin-2-yl)piperidin-4-yl]-4H-[1,2,4]triazol-3-yl]methyl]methylamino]ethyl]pheny l]amine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of triazoles as vasopressin receptor V1a antagonists for treating of dysmenorrhea)

RN 748806-15-7 CAPLUS

CN 4H-1,2,4-Triazole-3-methanamine, N-[1-(2-amino-5-chlorophenyl)ethyl]-4-(4-chlorophenyl)-N-methyl-5-[1-(2-pyrimidinyl)-4-piperidinyl]- (CA INDEX NAME)



THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/588,876

=> log y	
COST IN U.S. DOLLARS	
FULL ESTIMATED COST	

SINCE FILE TOTAL ENTRY SESSION 11.38 190.41

SINCE FILE TOTAL
ENTRY SESSION
-1.60 -1.60 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 14:57:30 ON 07 JAN 2008